

# QUANTITATIVE TECHNIQUE FOR COMPARING SIMULANT MATERIALS THROUGH FIGURES OF MERIT. Doug Rickman<sup>1</sup>, Hans Hoelzer<sup>2</sup>, Kathy Fourroux<sup>3</sup>, Charles Owens<sup>4\*</sup>, Carole McLemore<sup>5\*</sup>, John Fikes<sup>6</sup>,

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**Introduction:** The 1989 workshop report entitled *Workshop on Production and Uses of Simulated Lunar Materials* [1] and the *Lunar Regolith Simulant Materials: Recommendations for Standardization, Production, and Usage*, NASA Technical Publication [2] both identified and reinforced a need for a set of standards and requirements for the production and usage of the Lunar simulant materials. As NASA prepares to return to the Moon, and set out to Mars a set of early requirements [3] have been developed for simulant materials and the initial methods to produce and measure those simulants have been defined. Addressed in the requirements document are: 1) a method for evaluating the quality of any simulant of a regolith, 2) the minimum characteristics for simulants of Lunar regolith, and 3) a method to produce simulants needed for NASA's Exploration mission. As an extension of the requirements document a method to evaluate new and current simulants has been rigorously defined through the mathematics of Figures of Merit (FoM).

A single FoM is conceptually an algorithm defining a single characteristic of a simulant [4] and provides a clear comparison of that characteristic for both the simulant and a reference material. Included as an intrinsic part of the algorithm is a minimum acceptable performance for the characteristic of interest. The algorithms for the FoM are also explicitly keyed to a recommended method to make the simulants.

**Benefits for this approach;** 1) permit multiple materials to be used as standards or reference; 2) allow multiple simulants to be compared in a standardized manner; 3) allows simulants to be standardized to a definition based on measurement protocols and not restricted to a physical reference material; 4) new batches of simulants or multiple providers of simulants can be readily compared, and 5) simulant requirements are permitted to evolve as knowledge or needs change.

**Intended Users of the FoM:** The scientific and engineering communities are the primary two intended users of simulant materials and the data provided by the Figures of Merit.

Utilization of the simulant by the science community will be in small quantities (kilograms vs. metric tons in most cases) in a laboratory or specialized pilot facility with the intent of developing or improving a

process (e.g. oxygen or metals extraction) and may only require discrete amounts of simulant. Expectations are that the FoMs for these simulants will have higher values and tighter tolerances banding together to require more closely controlled simulant production techniques. This in turn reflects on the additional quality control aspects of how the simulant materials were collected, processed, and blended.

Potential simulant providers may use offsite analytical techniques to verify the simulant to the FoMs applied. "Offsite" implies that statistically relevant samples have been taken from the simulant components individually and the simulant after mixing, and analyzed in a laboratory setting to verify the quality of the product. Tighter production tolerances or secondary processing are expected to drive higher dollar/kg costs to the end user.

Utilization of the simulant by the engineering community will be in larger quantities (metric tons) necessary to develop large-scale processes for Lunar or Martian production facilities and construction. Examples of engineering uses include developing drills and excavation equipment along with handling and hauling mass quantities of regolith. Processes developed for Lunar or Martian industrial applications must be robust enough to handle small amounts of contamination inherent in the processing of large quantities of rocks and minerals on Earth. Many of these contaminants will be introduced during Lunar or Martian processing as well. Expectations are that the FoMs for these simulants will have lower values for some characteristics based on their intended end use. Potential vendors may use insite analytical techniques to verify quality of the simulant during production. "Insite" implies that a continuous sampling and analysis is occurring during the production run. Common methods of measurement utilized in continuous industrial processing are laser diffraction and automated vision systems. Automated analytic techniques coupled with large quantity production are expected to reduce the dollar/kg costs to the end user.

**Establishing Requirements Through the Figures of Merit:** Based on the work published in the *Lunar Regolith Simulant Materials: Recommendations for Standardization, Production, and Usage*, NASA Technical Publication [2], four key characteristics of

the Lunar regolith have been initially selected for the Simulant Requirements Document. Those characteristics are; composition, size, shape and density. As needs change new requirements and FoMs may be added, deleted or modified. To demonstrate the link between a Figure of Merit and requirements, the FoM of "composition" is used as an example.

The Figure of Merit termed "composition" defines the geologic constituents of the simulant without reference to textural features, such as particle shape and particle size. Composition includes the following classes of constituents: lithic fragments, mineral grains, glasses and agglutinates. Conceptually, composition addresses the chemical makeup of individual particles. The Simulant Requirements Document specifies the rock types, their chemical make up and which materials may or may not be used to establish a simulant requiring this type of Figure of Merit.

**Establishing a Reference Material:** In normal use a reference material would be defined as a regolith core sample returned by an Apollo mission. However, any material real or predicted may be used, including another simulant. The reference material is measured and assigned values of 1 for all properties to be described by the Figures of Merit. The simulant is measured for the same properties as the referenced material and the differences are evaluated according to the algorithms of the FoMs selected for comparison.

The usefulness of allowing a predicted material to be the reference is that as mission planners evaluate and select potential Lunar sites for exploration, existing and new simulants may be evaluated for potential analogs for those sites through the Figures of Merit. If simulants must be produced, manufacturers of such materials now have a way to measure their product and select the "best fit" of raw materials and processing techniques.

**Conclusions:** Requirements and techniques have been developed that allow the simulant provider to compare their product to a standard reference material through Figures of Merit. Standard reference material may be physical material such as the Apollo core samples or material properties predicted for any landing site. The simulant provider is not restricted to providing a single "high fidelity" simulant, which may be costly to produce. The provider can now develop "lower fidelity" simulants for engineering applications such as drilling and mobility applications.

**References:** [1] D. S. McKay, James D. Blacic, *Workshop on Production and Uses of Simulated Lunar Materials*, LPI Technical Report Number 91-01. [2] Sibille L., Carpenter P., Schlagheck R., and French R. (2005) *Lunar Regolith Simulant Materials: Recommendations for Standardization, Production, and Usage*, NASA Technical Publication NASA/TP-2006-

214605. [3] Marshall Space Flight Center, *Lunar Regolith Simulant Requirements*, MSFC-RQMT-3503, March 1, 2007. [4] *A Quantitative Method For Evaluating Regolith Simulants*, D. Rickman, H. Hoelzer, P. Carpenter, L. Sibille, R. Howard, C. Owens, Space Technology & Applications International Forum (STAIF-2007), University of New Mexico, Feb 2007.

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# Quantitative Techniques for Comparing Simulant Materials through Figures of Merit

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# Agenda

- A quick review of Figures-of-Merit.
  - Composition
  - Size distribution
  - Shape
  - Density
- Software Implementation of FoM Algorithms.
  - Components of the software
  - Inputs to the software
- Demonstration of the software.
- Backup slides.



A composite image of Earth, the Moon, and the Sun in space. The Earth is in the lower-left foreground, showing blue oceans and white clouds. The Moon is in the center, partially obscured by the Earth. The Sun is in the background, a large, glowing orange-yellow sphere. The text "A Quick Review of Figures-of-Merit" is centered over the image in white.

# A Quick Review of Figures-of-Merit

# Characterization of Simulant Materials

- A method is needed to specify simulant requirements and simulant suitability for a given purpose and to compare different simulants and simulants to reference materials.
- D. Rickman has postulated that a simulant may be characterized by the following four quantities:
  - material composition
  - particle size distribution
  - particle shape
  - material density
- This leads to the search for methods of specifying and comparing materials in terms of these four quantities.



## Figures of Merit (FoM)

- A FoM is conceptually an algorithm for quantifying a single characteristic of a simulant and provides a clear measure of how well a simulant and reference material compare.
- The human mind can only compare and rank scalars. Thus to compare more complex quantities, a method (algorithm) must be devised which boils the complex quantity down to a scalar.
- In our context a FoM is a measure of how well a characteristic of a simulant material compares to a reference material.
- For simulant specification and comparison, there are four FoMs, for the quantities *composition*, *size*, *shape* and *density*.

# Composition

- Composition defines the geologic constituents of a simulant without reference to textural features, such as particle shape and particle size.
- Composition includes the following classes of constituents:
  - lithic fragments
  - mineral grains
  - glasses
  - Agglutinates
- Conceptually, composition addresses the chemical makeup of individual particles.
- Composition may be a function of the size of the particles.



# Size Distribution

- Size distribution refers to the distribution of particle sizes.

# Shape

- Measures for Shape are still under development but may include:
  - Mean Width
  - Mean Shape Factor
  - Mean Aspect Ratio
  - Convexity
- A Figure of Merit for shape is still under development and may influence how shape is defined and measured.

# Density

- Density refers to the average weight per unit volume of a material.



## Figures of Merit Usage

- The FoMs have been constructed to lie in the range 0 to 1 with 0 indicating a poor or no match and 1 indicating a perfect match.
- The FoM may be used for specification by stating the value a simulant's FoM must attain in order to be suitable for a given application.
  - as an example, for composition, an FoM of .75 might be quite suitable for road building experiments, while an FoM of .98 might be required for chemistry experiments
- The FoM methodology may be used to compare various simulants from different vendors, production runs, and different kinds of simulant.
- The FoM of a simulant may be used during production for quality control.

# Algorithms for the FoMs - Some Preliminaries

## Reference Material

- Reference material refers to the *desired* composition, size, shape or density of a material.
- The composition, size, shape or density of a reference material usually mirrors that of an actual material but does not have to.
  - a reference material may be completely hypothetical
- As such a reference material may be used for specification of a simulant.
- A simulated material may also be compared to the reference material.
  - the simulated material should match to the degree specified, the reference material



# Composition

- The composition of a material (reference or simulant) is defined as a *vector* of the fraction of the various constituents of the material.
- Composition may be defined at multiple levels of granularity, starting with the composition in terms of the four basic classes of constituents, lithic fragments, minerals, glasses and agglutinates.
  - each class may be sub-divided into sub-constituents as necessary for a particular application
  - this process may be repeated for multiple levels, but the level of detail need not be uniform across the various classes and sub-constituents or between two materials
  - the elements of a composition vector must necessarily sum to unity (the sum of the fractional parts must equal the whole) excluding contaminants
- Composition may also be defined as a function of size, so that a composition definition for a substance consists of a set of vectors for various different particulate sizes, one vector for each of the various particle sizes or range of particle sizes.



# Composition FoM

- The Figures of Merit is defined as the scaled L1 norm of the difference of two composition vectors subtracted from unity.
- Scaling (normalization) forces the norm of the difference of two composition vectors to lie between 0 and 1, and subtraction from unity results in a figure of merit of 1 for a perfect match to 0 for no match at all (as opposed to the other way around).

$$FoM = 1 - \frac{\left\| w_{adjusted} \left( C_{adjusted\ reference} - C_{adjusted\ simulant} \right) \right\|_1}{\left\| \begin{bmatrix} \max_1(w_{adjusted}) & \max_2(w_{adjusted}) \end{bmatrix} \right\|_1}$$

$$= 1 - \frac{\sum_i w_{adjusted_i} \left| C_{adjusted\ reference_i} - C_{adjusted\ simulant_i} \right|}{\max_1(w_{adjusted}) + \max_2(w_{adjusted})}$$

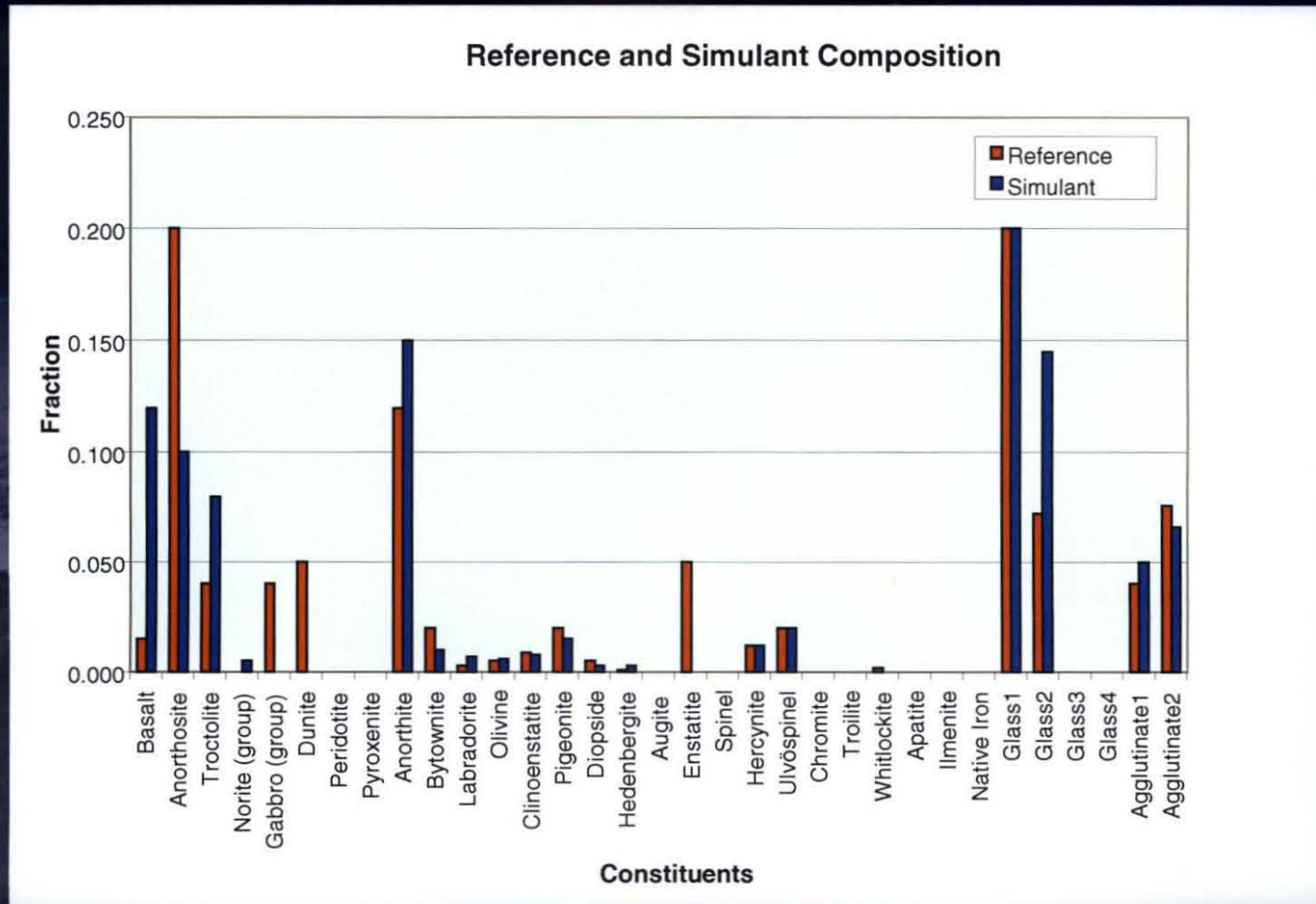
$\|w\|_1$  denotes the L1 norm of vector  $w$

$\max_i(w)$  is  $i^{th}$  largest element of  $w$

- The L1 norm of a vector is defined as the sum of the absolute values of the elements of the vector.

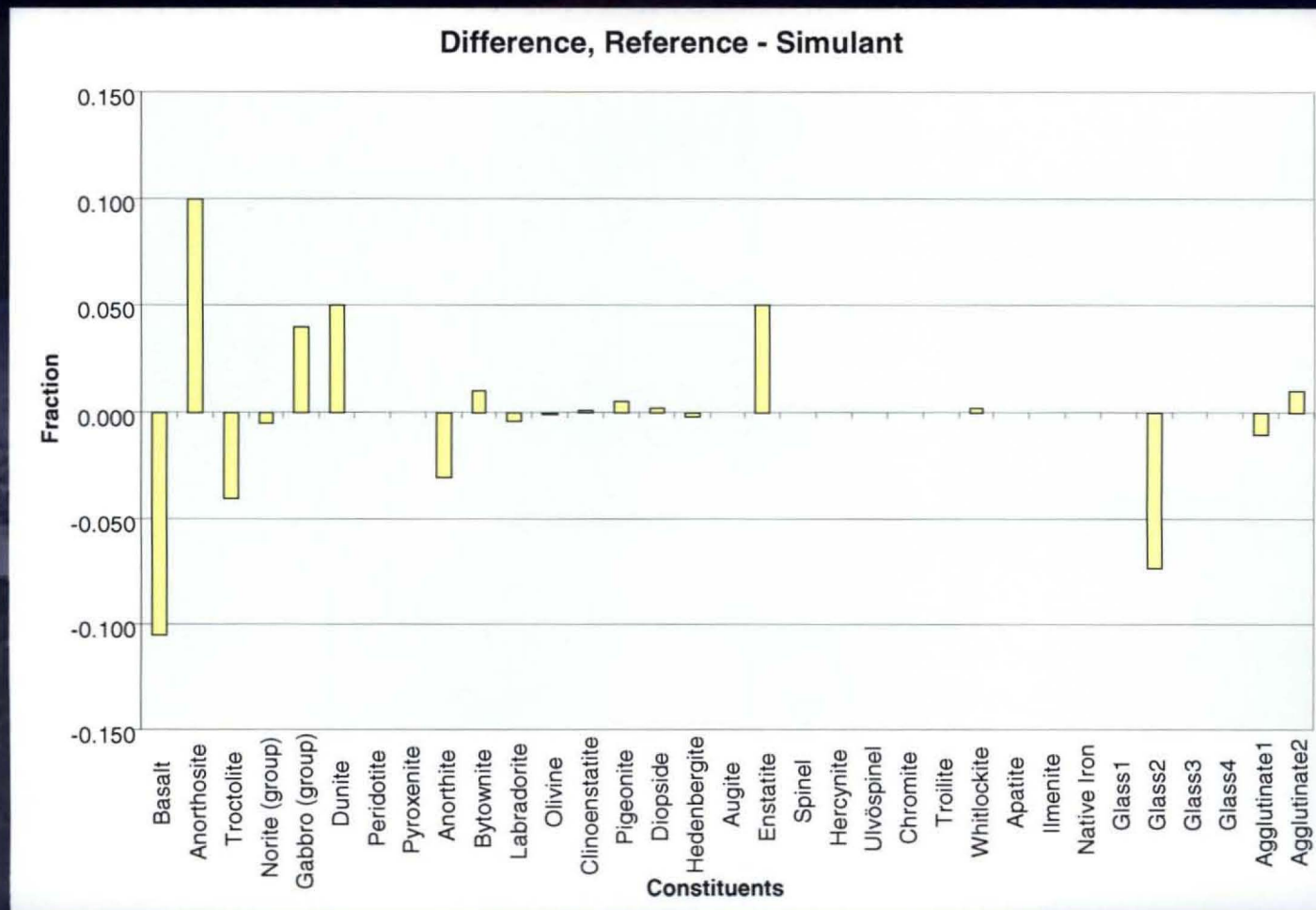
# Composition FoM

## Composition vectors displayed as a bar chart (example)



# Composition FoM

## Difference of composition vectors (example)





## Size Distribution FoM

- The FoM for a given reference and simulant relative frequency distributions is defined as 1 minus the square root of the integral of the weighted difference of the RFDs squared divided by the sum of the weighted integrals of the squares of the individual RFDs.

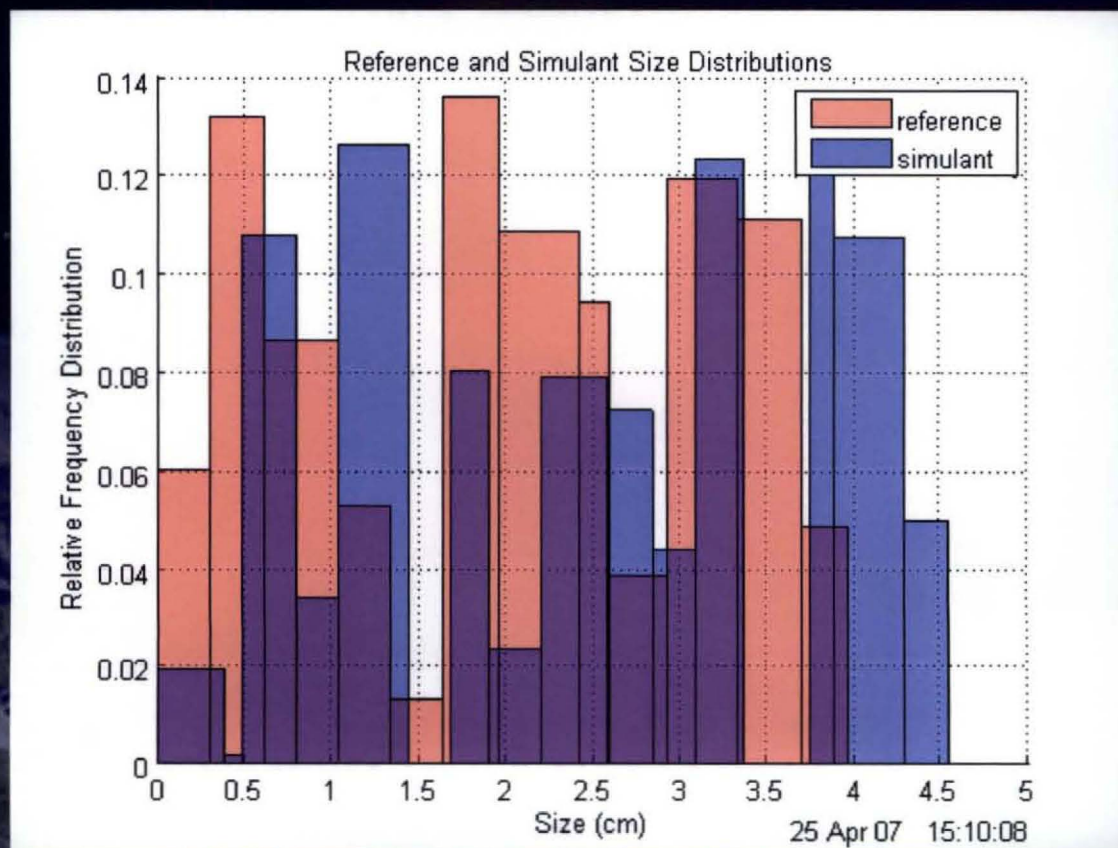
$$FoM_{before\ constraints} = 1 - \frac{\sqrt{\int w (RFD_{reference} - RFD_{simulant})^2}}{\sqrt{\int w RFD_{reference}^2 + \int w RFD_{simulant}^2}}$$

- The FoM is further subject to certain maximum error constraints:

$$FoM = \begin{cases} FoM_{before\ constraints} & \text{if } |RFD_{reference} - RFD_{simulant}| \leq \max RFD \text{ difference} \\ 0 & \text{otherwise} \end{cases}$$

# Size Distribution FoM

## Histogram of relative frequency as a function of size





# Density

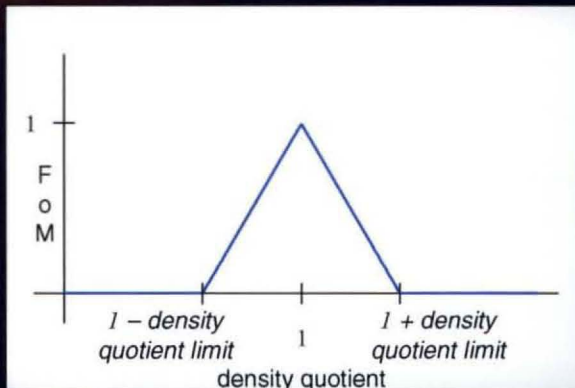
- Density refers to the average weight per unit volume of a material.
- Density shall be measured by taking a sufficiently large enough sample so that the sample follows the particle size distribution of the material as defined in the slides on Size Distribution.
  - This avoids biasing the value of the density to the density of an aggregate of small particles which may pack more closely or an aggregate of large particles which may pack more loosely than an aggregate of particles which follows the particle size distribution as defined in the slides on Size Distribution.



# Density FoM

- The figure of merit for how closely a simulant matches a reference is proportional to the ratio of the densities.
- Ratios of less than  $1 - \text{density quotient limit}$  or greater than  $1 + \text{density quotient limit}$  correspond to figures of merit of 0, while a ratio of 1 corresponds to a figure of merit of 1.
- Mathematically and graphically this may be expressed as:

$$FoM = \begin{cases} \frac{1}{\text{density quotient limit}} \left( \frac{\text{simulant density}}{\text{reference density}} \right) + \frac{\text{density limit} - 1}{\text{density quotient limit}} & \text{for } 1 - \text{density quotient limit} \leq \frac{\text{simulant density}}{\text{reference density}} < 1 \\ \frac{-1}{\text{density quotient limit}} \left( \frac{\text{simulant density}}{\text{reference density}} \right) + \frac{\text{density limit} + 1}{\text{density quotient limit}} & \text{for } 1 \leq \frac{\text{simulant density}}{\text{reference density}} < 1 + \text{density quotient limit} \\ 0 & \text{otherwise} \end{cases}$$



The background of the slide is a deep space scene. In the lower-left foreground, a portion of the Earth is visible, showing blue oceans and white cloud patterns. Behind it, the grey, cratered surface of the Moon is partially visible. In the upper-middle background, there is a large, glowing nebula or galaxy with vibrant orange, yellow, and blue hues. The rest of the background is a dark, star-filled space.

# Software Implementation of FoM Algorithms



# Components of the Software

The software which implements the Figures-of-Merit consist three parts:

- An input editor – we use Microsoft Excel for this purpose.
- A back end that computes the Figures-of-Merit – we use The MathWorks Matlab for this purpose.
- A front end with which the user interacts that opens and reads the Excel input files, performs checks on the inputs and calls the Matlab routines for computation of the FoMs – This is custom code.



## What the FoM Software Is and Is Not

- Given input data on the composition, size distribution, shape and density of two materials, the FoM software computes the Figures-of-Merit discussed in this presentation.
- The software itself DOES NOT contain any data; it is not a database, only a computational engine.

# Inputs - Composition

Microsoft Excel - FDM Template.xls

File Edit View Insert Format Tools Data Window Help Design Sheet

Type a question for help

AX37

Composition		Size Range 1		Size Range 2		Size Range 3		Size Range 4		Size Range 5		Size Range 6		Size Range 7		Size Range 8		Units	
		lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit		
1	Composition																		
2																			
3	Short Instructions																		
4																			
5																			
6																			
7	Sum of Components																		
8	(computed - must sum to unity)																		
9																			
10	Lithic Fragments	0.000		0.000		0.000		0.000		0.000		0.000		0.000		0.000			
11	Total (no further breakdown)																		
12	Basalt																		
13	Anorthosite																		
14	Troctolite																		
15	Norite (group)																		
16	Gabbro (group)																		
17	Dunite																		
18	Pseudotachylite																		
19	Pyroxenite																		
20	Mineral Grains	0.000		0.000		0.000		0.000		0.000		0.000		0.000		0.000			
21	Total (no further breakdown)																		
22	Anorthite																		
23	Bytownite																		
24	Labradorite																		
25	Olivine																		
26	Clinoenstatite																		
27	Pigeonite																		
28	Diopside																		
29	Hedenbergite																		
30	Augite																		
31	Enstatite																		
32	Spinel																		
33	Hercynite																		
34	Ulvöspinel																		
35	Chromite																		
36	Troilite																		
37	Whitlockite																		
38	Apatite																		
39	Ilmenite																		
40	Native Iron																		
41	Glasses	0.000		0.000		0.000		0.000		0.000		0.000		0.000		0.000			
42	Total (no further breakdown)																		
43	Glass1																		
44	Glass2																		
45	Glass3																		
46	Glass4																		

Ready

Composition / Size Distribution / Shape / Density

Short Instructions

For up to 8 Size Ranges, enter the following data (a Figure for each Size Range):

- 1) The lower and upper limits (e.g., 25, 50).
- 2) The units for the sizes (e.g., micrometer).
- 3) The fraction of each component. If only level A composition is specified, enter the fraction (no further breakdown).
- 4) For Reference sample component should be specified. These fields are not used.
- 5) For Glasses and Agglutines, etc. with a more detailed breakdown.

Note: Only fractions at the higher levels are computed.



# Inputs – Size Distribution

Microsoft Excel - FOM Template.xls

File Edit View Insert Format Tools Data Window Help Design Sheet

Type a question for help

AK36

1	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
2	<b>Particle Size Distribution</b>																		
3		Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Bin 9	Bin 10	Bin 11	Bin 12	Bin 13	Bin 14	Bin 15	Bin 16		
4	Lower Bin Size																		
5	Bin Size Units																		
6	Fraction*																		
7	Importance																		
8																			
9	*Sum of fractions																		
10	(must sum to unity)																		
11																			
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Legend

input fields

Units

μm micrometer 10<sup>-6</sup> meter (m)

mm millimeter 10<sup>-3</sup> meter (m)

cm centimeter 10<sup>-2</sup> meter (m)

**Short Instructions**

For as many Bins as desired (columns B, C, D, etc.) enter the following data:

- 1) The size of the lower end of a Bin (e.g. for a Bin spanning the size range 50 to 100, 50 would be entered). Bins will be treated as contiguous, so that the upper end of a Bin will be the lower end of the next Bin.
- 2) The units for the sizes specified in step 1. (e.g. microns, mm).
- 3) The fraction of particles of the total in this size Bin.
- 4) For Reference samples, the relative importance of the component should be specified. For simulant samples, these fields are not used.

Note: For n Bins, n + 1 sizes must be specified

Note: Fractions should sum to unity over all Bins

Ready



## Inputs - Shape

Microsoft Excel - FQM Template.xls

Type a question for help

File Edit View Insert Format Tools Data Window Help Design Sheet

AW29

Particle Shape

Size Range 1  
lower upper  
limit limit

Size Range 2  
lower upper  
limit limit

Size Range 3  
lower upper  
limit limit

Size Range 4  
lower upper  
limit limit

Size Range 5  
lower upper  
limit limit

Size Range 6  
lower upper  
limit limit

Size Range 7  
lower upper  
limit limit

Size Range 8  
lower upper  
limit limit

Units

μm micrometer 10<sup>-6</sup> meter (m)

mm millimeter 10<sup>-3</sup> meter (m)

cm centimeter 10<sup>-2</sup> meter (m)

Mean Width

Mean Shape Factor

Mean Aspect Ratio

Convexity

Short Instructions

For up to 8 Size Ranges, enter the following data (a Figure-of-Merit (FOM) will be computed for each Size Range).

1) The lower and upper limits of the size range (e.g. 0, 100, 25, 50).

2) The units for the sizes specified in step 1. (e.g. microns, mm).

3) Mean Width - use units specified for size ranges.

4) Mean Shape Factor =  $\text{perimeter}^2 / 4 \times \text{area}$

5) Mean Aspect Ratio = length / width

Legend

input fields

Composition Size Distribution Shape Density

Ready

# Inputs - Density

Microsoft Excel - FOM Template.xls

File Edit View Insert Format Tools Data Window Help Design Sheet

Type a question for help

AJ46

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Density																
2				units													
3	density			g/cm <sup>3</sup>													
4	units			kg/m <sup>3</sup>													
5																	
6																	
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Short Instructions

Enter the following data:

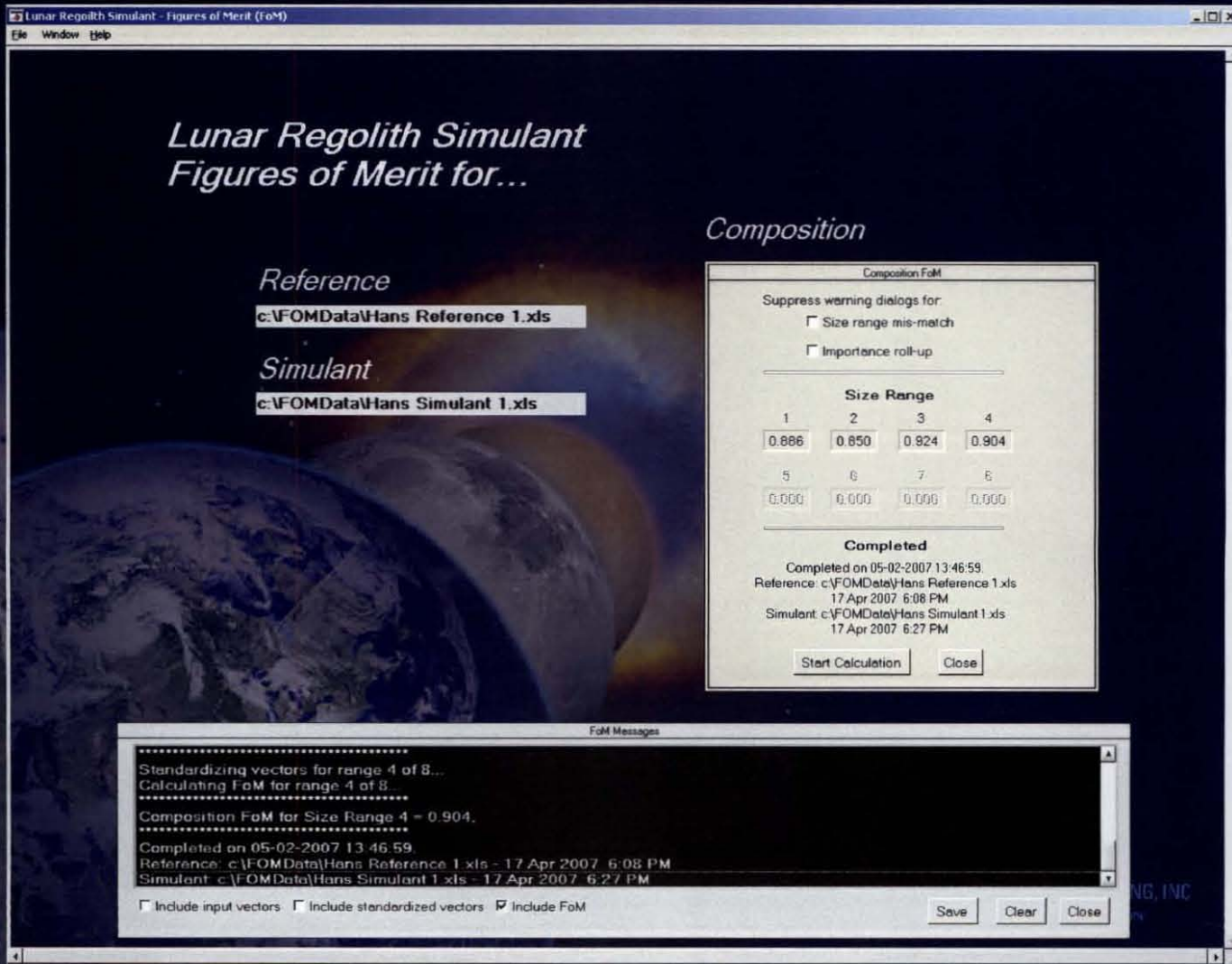
- 1) The density of the sample
- 2) The units for the density

Legend

input fields

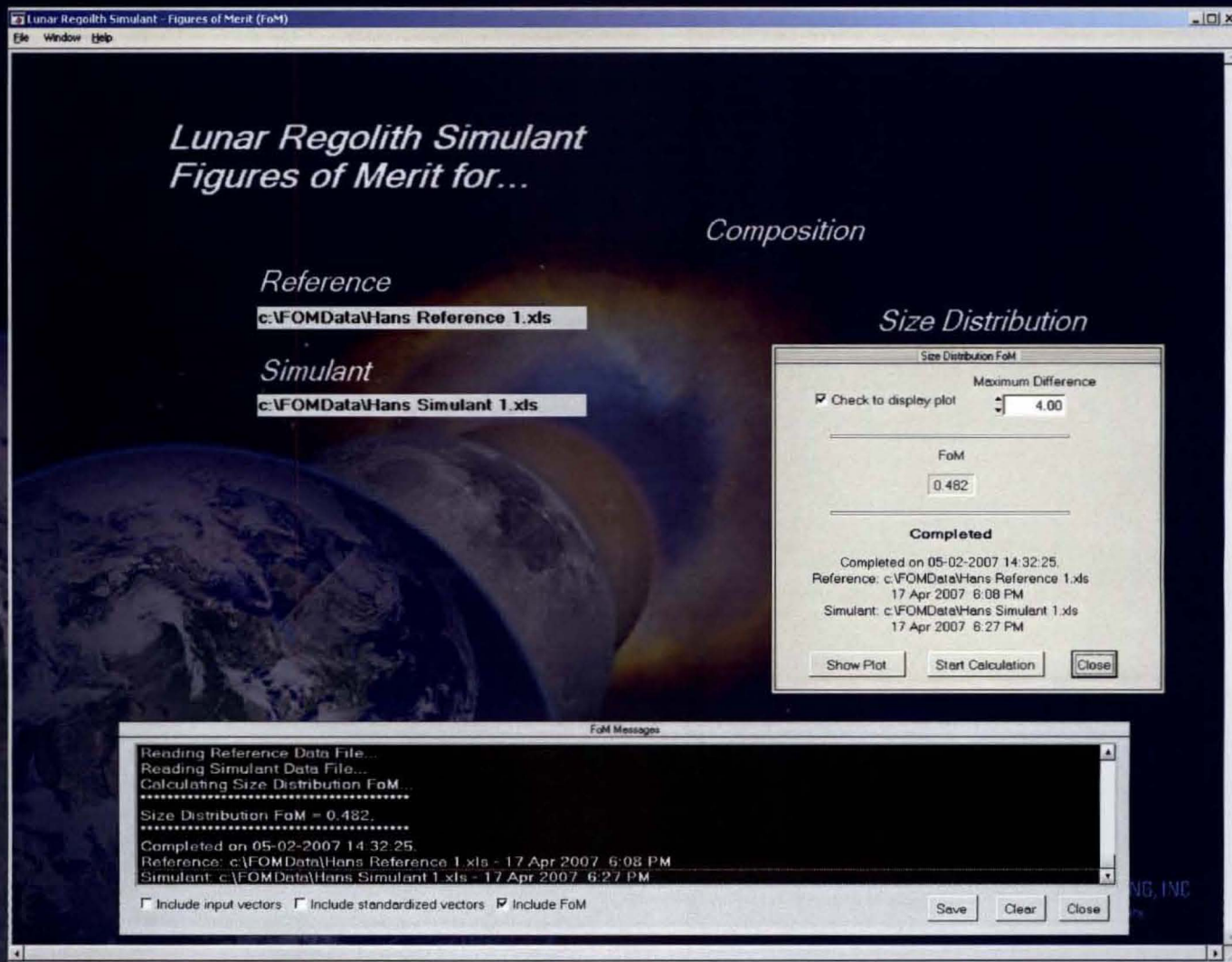
Ready

# FoM – Composition

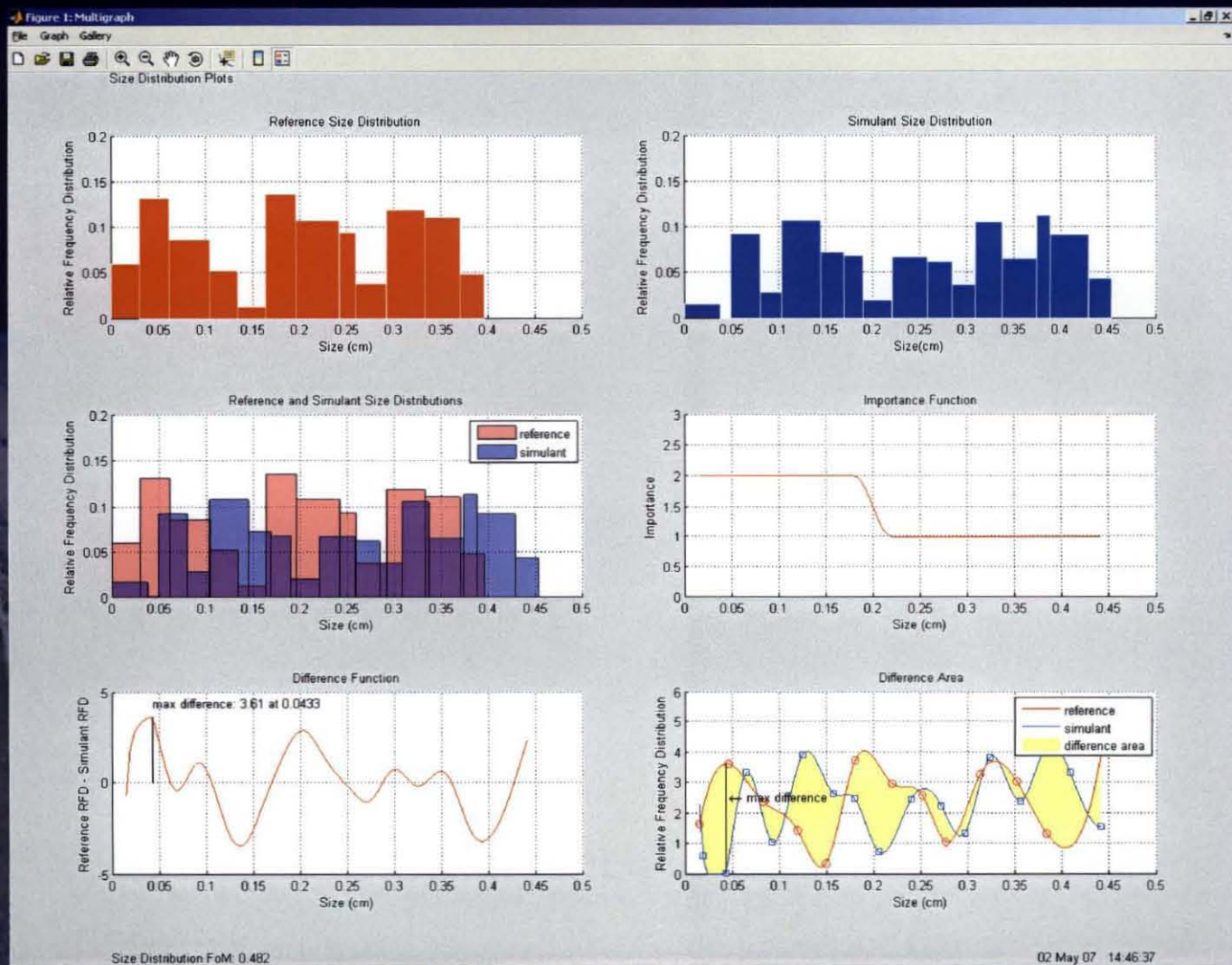




# FoM – Size Distribution - 1



# FoM – Size Distribution - 2





# FoM – Density





A composite image of Earth, the Moon, and a rainbow in space. The Earth is in the bottom left, showing continents and clouds. The Moon is in the center, partially obscured by the rainbow. The rainbow is a vibrant arc of colors in the dark blue/black background of space. The text "Backup Slides" is centered over the image in a white, sans-serif font.

# Backup Slides

# Regolith Properties To Be Simulated And Their Relationship to the Figures Of Merit

Simulant Properties \ Figures of Merit	Composition	Size	Shape	Density
<b>1. Grain Properties</b>	X	X	X	
<b>2. Electrostatic Charging Properties</b>	X	X		
<b>3. Magnetic Properties</b>	X	X		
<b>4. Geomechanical Mechanical</b>				
<b>a. Fatigue</b>	X	X	X	X
<b>b. Strength</b>				
<b>i. Tensile</b>	X	X	X	X
<b>ii. Compressive</b>	X	X	X	X
<b>iii. Shear</b>	X	X	X	X
<b>iv. Grain Hardness</b>	X			
<b>v. Coefficient of Friction</b>	X	X	X	X
<b>c. Flexural Strength – Bending Resistance</b>	X	X	X	X
<b>d. Fracture Properties</b>	X	X	X	X
<b>e. Impact Resistance</b>	X	X	X	X
<b>f. Rheology (flow properties)</b>	X	X	X	X
<b>g. Angle of Repose</b>		X	X	X

# Regolith Properties To Be Simulated And Their Relationship to the Figures Of Merit

Simulant Properties \ Figures of Merit	Composition	Size	Shape	Density
<b>4. Geomechanical (cont'd)</b>				
<b><u>Physical</u></b>				
h. Thermal Properties	X	X	X	X
i. Bulk Density	X	X	X	
j. Particle Density	X			
k. Porosity	X	X	X	X
l. Surface Area	X	X	X	
m. Permeability (gas)	X	X	X	X
<b>5. Agglutinate-specific</b>				
a. Friability				
b. With single-domain iron				
<b>6. Chemical Reactivity</b>				
a. From surface damage				
b. As volatile / soluble minerals				
<b>7. Chemical Properties</b>				
a. Bulk	X	X	X	X
b. Mineral	X	X	X	



# Regolith Properties To Be Simulated And Their Relationship to the Figures Of Merit

Figures of Merit Simulant Properties	Composition	Size	Shape	Density
<b>7. Chemical Properties (cont'd)</b>				
c. Glass	X	X	X	
<b>8. Modal Composition</b>				
a. Total	X			
b. As a function of grain size		X		
<b>9. Texture</b>	X	X	X	
<b>10. Implanted solar particle-specific (e.g. H, C, N)</b>	X			